Thermal Crossover between Ultrasmall Double and Single Junction

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The crossover from double-junction behavior to single-junction behavior of ultrasmall tunnel junctions is studied theoretically in a scanning-tunneling microscope setup. The independently variable tip temperature of the microscope is used to monitor the transition between both regimes.

73.23.Hk, 73.40Gk, 73.40Rw

I. INTRODUCTION

The Coulomb blockade of the current through a system of ultrasmall tunnel junctions is one of the basic features of single electronics. There are two simple systems capable of producing this blockade if connected to a voltage source, namely the single junction within a high-impedant environment and the double junction. Owing to their different features the theoretical description of the former is much more simple than that of the latter, whereas manufacturing favors the latter instead of the former.

In this paper we study theoretically the crossover from double-junction behavior to single-junction behavior in the usually scanning-tunneling-microscope setup.[2] The tip junction, i.e. where the outer electrode is formed by the microscope tip, is characterized by the resistance R_1 and the capacitance C_1, whereas the corresponding parameters of the other junction are denoted R_2 and C_2. The crossover between double-junction regime and single-junction regime is governed by the temperature of the microscope tip, $T_{\rm tip}$, which is thought to be independent of the temperature of the other electrodes, $T_{\rm base}$. We discuss the case $T_{\rm tip} \geq T_{\rm base}$ only. In order to observe a Coulomb blockade the base temperature is restricted to values $T_{\rm base} \ll E_{\rm C}/k_{\rm B}$, where $E_{\rm C} = 1/2\, e^2/(C_1 + C_2)$ is the Coulomb energy of the double junction.

If the tip temperature is comparable to the base temperature, a usual double-junction behavior is expected. Its theoretical description is the so-called "orthodox theory":[3,4] a master equation describes the occupation probability of different charge states of the small island between the two junctions. The current through the system is expressed in terms of these probabilities.

If the tip temperature is well above $T_{\rm base}$, thermal fluctuations will make the tip junction more transparent. However, its resistance is still large on the scale of the quantum resistance $R_{\rm k} = {\rm h}/e^2 \approx 25.8{\rm k}\Omega$. Thus we have the typical single-junction setup: an ultrasmall tunnel junction at base temperature and an high impedant almost ohmic environment resistance. The small capacitance of the latter is negligible.

This paper is organized as follows. The theoretical approximations for our discussion are given in the next Section. After this follow the discussion itself and the conclusion.

II. THEORETICAL DESCRIPTION

A. Double junction

The ultrasmall double junction is described in terms of standard "orthodox theory".[3,4] Assuming the tunnel rates through the first (1) and second (2) junction in right (r) and left (l) direction are known as $r_{1,2}(n)$ and $l_{1,2}(n)$ for n extra charges on the central island, the time dependence of the occupation probability $\sigma(n)$ of the state n follows from the master equation[3,4]

$$\begin{aligned}\frac{{\rm d}\sigma(n,t)}{{\rm d}t} &= \big[r_1(n-1) + l_2(n-1)\big]\sigma(n-1,t) \\ &\quad + \big[r_2(n+1) + l_1(n+1)\big]\sigma(n+1,t) \\ &\quad - \big[r_1(n) + r_2(n) + l_1(n) + l_2(n)\big]\sigma(n,t).\end{aligned} \tag{1}$$

For the considered stationary situation we use the stationary solution of this equation[4,5]

$$\begin{aligned}\sigma(n) &= \frac{1}{\mathcal{Z}} \prod_{i=-\infty}^{n-1} \big[r_1(i) + l_2(i)\big] \\ &\quad \times \prod_{j=n+1}^{\infty} \big[r_2(j) + l_1(j)\big]\end{aligned} \tag{2}$$

with an appropriate normalization $\mathcal{Z}$ so that

$$\sum_{n=-\infty}^{\infty} \sigma(n) = 1.$$

The stationary average current results from $\sigma(n)$

$$\begin{aligned}\langle I \rangle &= e \sum_{n=-\infty}^{\infty} \big[r_1(n) - l_1(n)\big]\sigma(n) \\ &= e \sum_{n=-\infty}^{\infty} \big[r_2(n) - l_2(n)\big]\sigma(n).\end{aligned} \tag{3}$$

Let us consider the transition rates $r_{1,2}(n)$ and $l_{1,2}(n)$ in detail now. They depend on n via the energy differences $E_{1,2}^{r;l}(n)$ caused by the respective tunneling event,

$$E^r_{1,2}(n) = E_\mathrm{C}\big(\frac{C_{2,1}V}{e} \mp n - \frac{1}{2}\big) \qquad (4)$$
$$E^l_{1,2}(n) = E_\mathrm{C}\big(-\frac{C_{2,1}V}{e} \pm n - \frac{1}{2}\big).$$

If the electron temperature on both sides of the junction is the same, Fermi's Golden Rule results in[3,4]

$$\{r,l\}_{1,2}(n) = \frac{1}{e^2 R_{1,2}} \frac{E^{r,l}_{1,2}(n)}{1-\exp[-\beta_\mathrm{base} E^{r,l}_{1,2}(n)]}, \qquad (5)$$

where $\beta_\mathrm{base} = (k_\mathrm{B} T_\mathrm{base})^{-1}$ is used. In case of considerably different temperature on both sides of the junction we use instead[6]

$$\{r,l\}_{1,2}(n) = \frac{k_\mathrm{B} T_\mathrm{tip}}{e^2 R_{1,2}} \log\left[\exp\left(\frac{E^{r,l}_{1,2}(n)}{k_\mathrm{B} T_\mathrm{tip}}\right) + 1\right]. \qquad (6)$$

As shown in Ref. 6, (6) is a reasonable approximation for $T_\mathrm{tip} \geq 2T_\mathrm{base}$. Eq. 6 indicates that the tunneling behavior in this case is governed by the higher temperature. The influence of the temperature difference results in the change of (6) in comparison to (5).

B. Single junction

Since the single-junction regime requires a warm tip we consider the hot environment only. In this case the energy excitation probability of the environment $P(E)$ is given by a Gaussian[7]

$$P(E) = \frac{1}{2}\sqrt{\frac{\beta_\mathrm{env}}{\pi E_\mathrm{c}}} \exp\left[-\frac{\beta_\mathrm{env}}{4E_\mathrm{c}}(E-E_\mathrm{c})^2\right] \qquad (7)$$

where we introduced the single-junction charging energy $E_\mathrm{c} = e^2/(2C_2)$ and $\beta_\mathrm{env} = (k_\mathrm{B} T_\mathrm{env})^{-1}$ describes the elevated environment temperature. Eq. 7 fulfills the sum rules[8]

$$\int \mathrm{d}E\, P(E) = 1 \qquad (8)$$
$$\int \mathrm{d}E\, E\, P(E) = E_\mathrm{c}.$$

In Ref. 9 a Lorentzian shape is derived for the hot environment and negligible charging energy, but we have not found satisfactory results with that formula. In the considered temperature range charging effects are still essential as can be seen from the occurance of the Coulomb blockade. Hence, the situation here might be well outside the scope of the Lorentzian formula of Ref. 9.

The single junction at T_base is described by two rates, namely r_2 and l_2. Their functional dependence on the energy difference between both sides of the junction follows (5), but the energies $E^{r,l}_2$ are the voltage drops across the junction. For low base temperature we can make use of the approximation[10]

$$\frac{E}{1-\exp(-\beta E)} \approx E\Theta(E) + \frac{1}{\beta}\exp(-\gamma|E|)$$

with $\gamma = (6/\pi^2)\beta = 0.607\,927\beta$ from the normalization

$$\int_{-\infty}^{0} \frac{\mathrm{d}E\, E}{1-\exp(-\beta E)} = \frac{\pi^2}{6\,\beta^2} = \int_{-\infty}^{0} \frac{\mathrm{d}E}{\beta}\exp(-\gamma|E|).$$

This allows for an analytic expression of the current through the junction

$$I(V_2) = e\int \mathrm{d}E\, P(E)\big[r_2(eV_2 - E) - l_2(-eV_2 - E)\big],$$

where we use $E^{r,l}_2 = \pm eV_2 - E$. The current is calculated in terms of the voltage V_2 across the single junction, which does not include the voltage drop V_1 at the tip junction. Using $g = R_\mathrm{k}/R_1$ the final expression is

$$\begin{aligned} I(V_2) = \frac{V_2}{2R_2} + \frac{1}{e\,R_2}\Big\{ &-\frac{E_\mathrm{c}}{\pi}\arctan\frac{\beta_\mathrm{env} g}{2\pi}(eV_2 - E_\mathrm{c}) + \frac{eV_2 - E_\mathrm{c}}{\pi}\arctan\frac{\beta_\mathrm{env} g}{2\pi}(eV_2 + E_\mathrm{c}) \\ &+ \frac{1}{\beta_\mathrm{env} g}\log\frac{1+\big[\beta_\mathrm{env} g(eV+E_\mathrm{c})/(2\pi)\big]^2}{1+\big[\beta_\mathrm{env} g(eV-E_\mathrm{c})/(2\pi)\big]^2} \\ &+ \frac{4}{\beta_\mathrm{base}\beta_\mathrm{env}\gamma_\mathrm{base} g}\Big[\frac{1}{[2\pi/(\beta_\mathrm{env} g)]^2 + [eV_2 - E_\mathrm{c}]^2} - \frac{1}{[2\pi/(\beta_\mathrm{env} g)]^2 + [eV_2 + E_\mathrm{c}]^2}\Big]\Big\}. \end{aligned} \qquad (9)$$

For dominating bias, $eV_2 \gg E_\mathrm{c}, k_\mathrm{B} T_\mathrm{env}$, the asymptotic behavior $I(V_2) = (V_2 - E_\mathrm{c}/e)/R_2$ is recovered.

III. DISCUSSION

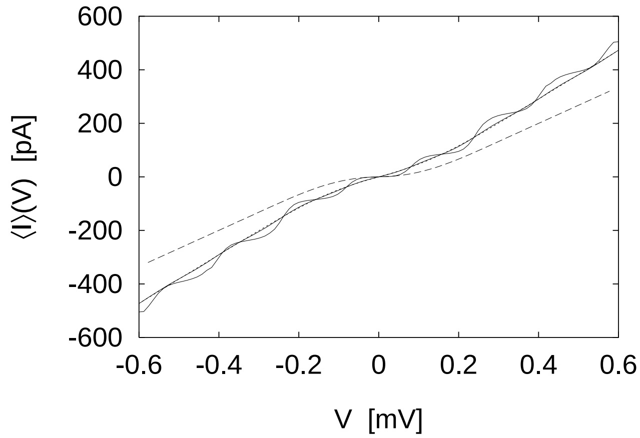

FIG. 1. Calculated current through an STM double junction ($C_1 = 1.0\text{fF}$, $C_2 = 0.1\text{fF}$, $R_1 = 1.0\text{M}\Omega$, $R_2 = 0.1\text{M}\Omega$, $T_{\text{base}} = 0.1\text{K}$) for tip temperature $T_{\text{tip}} = 0.2\text{K}$ (solid line, staircase) and $T_{\text{tip}} = 1.0\text{K}$ (solid line, straight). The long dashed line shows the result of a zero-temperature-environment calculation, whereas the short-dashed line displays Eq. 9 with $T_{\text{env}} = 0.75\text{K}$.

In Fig. 1 the result of our calculation are shown for the case of an asymmetric double junction. Double junction systems where an STM forms one junction are very often asymmetric. This asymmetry results in a Coulomb staircase as seen for the low temperature curve in Fig. 1. For higher tip temperature the stairs are smeared out, but the Coulomb blockade survives. This is the expected behavior of a single junction in a high-impedant environment. The curve is fitted well by our model of the hot environment and the derived current (9). The fit parameter is the temperature T_{env}, which is found between the low temperature T_{base} and the hot T_{tip}. Thus, it does not take wonder that the displayed zero-temperature approximation of $P(E)$ cannot describe the the double-junction system.

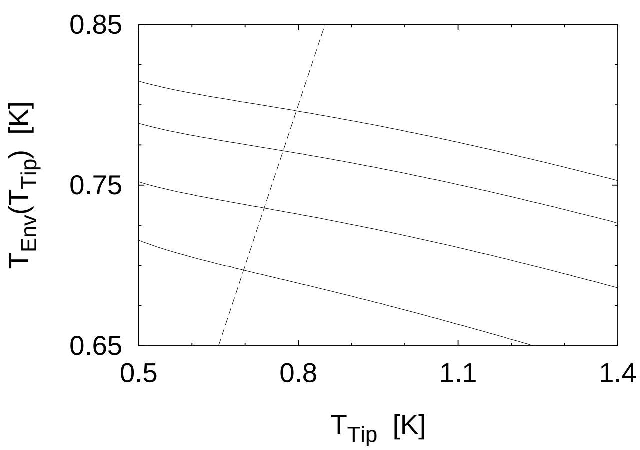

FIG. 2. The environment temperature T_{env} in dependence on the tip temperature T_{tip} for four different base temperatures $T_{\text{base}} = 0.05\text{K}$, 0.1K, 0.15K, 0.2K (from the top) as resulted from a least-square fit. The dashed line displays $T_{\text{env}} = T_{\text{tip}}$.

An interesting remaining question is the dependence of the environment temperature T_{env} on the choice of the base temperature T_{base} and the tip temperature T_{tip}. Since T_{env} is a theoretical parameter of our model we investigated this dependence by means of a fit procedure. The results (for the system of Fig. 1) are shown in Fig. 2. T_{env} is well above T_{base}, which corresponds to the results found in Ref. 6 for the single-electron electrometer. We restrict the consideration to the case $T_{\text{env}} \leq T_{\text{tip}}$. For low tip temperatures the Coulomb staircase makes a fit meaningless. The dependence on T_{tip} is weak. Nevertheless, it is astonishing that T_{env} decreases with increasing T_{tip} and increasing T_{base}. An rigorous treatment of the dependence of the (theoretical) environment temperature on the (real) base and tip temperature requires further investigation.

IV. CONCLUSION

In a theoretical treatment we have shown that the crossover between double-junction behavior and single-junction behavior in an STM setup can be monitored by a single parameter, the tip temperature of the STM. The tip junction works as an ohmic environment resistance for the hot tip. Even if the temperature on both sides of this junction is very different, its behavior can be described by an environment temperature alone.

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